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APPENDIX B

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McGraw-Hill Book Company
New York San Francisco Toronto London

electronic processes in materials

01/08/97 WED 15:46 FAX 1 508 795 5455

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ELECTRONIC PROCESSES IN MATERIALS

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distance along the a . Similarly, the length of b . The coordinates of all points are given in Table 4. One can proceed in a similar manner. In Fig. 22 are the coordinates of the points along the b . Since it is the coordinate along the b , the coordinate is $y\bar{x}$. The coordinate along the a is x . The symmetry-related points are shown in Fig. 22. The points are related to an *equipoint* set. The points are related to this set, its rank.

Two points at $\frac{1}{2}0$ are shown in Fig. 22. Since the points are "shared" by two unit cells, only two such points are shown in the unit cell. It is easy to see that the points are respectively, one. In the unit cell, there are special positions. The points can take on any position in the unit cell.

es of
points

$0, \bar{y}z$

3-dimensional space
obtained by adding
the points shown in Table 4.

Since the symmetry of $P4$ does not affect z , this coordinate is quite general for all equipoints. Note that Table 4 contains an additional column headed *Wyckoff notation*. This notation was proposed in one of the first tabulations of such data, and it has become common practice to refer to a position in a unit cell by its rank and letter.

Table 4
Equipoints of space group $P4$

Rank of equipoint	Wyckoff notation	Symmetry of location	Coordinates of equivalent points
1	a	4	$00z$
1	b	4	$\frac{1}{2}\frac{1}{2}z$
2	c	2	$0\frac{1}{2}z, \frac{1}{2}0z$
4	d	1	$xyz, y\bar{x}z, \bar{x}yz, \bar{y}xz$

The closest packings of spheres

Hexagonal and cubic closest packings. To a very close approximation, the atoms in crystals can be likened to hard impenetrable spheres. It is instructive, therefore, to consider some of the ways that spheres can be packed together in three-dimensional arrays. As a start, consider the arrangement of like spheres in a plane. An array in which the maximum available space is occupied is shown in Fig. 23A. This array is called a

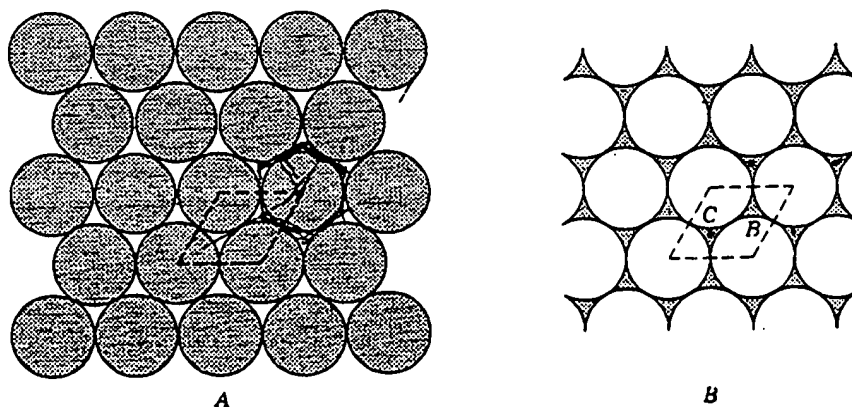


FIG. 23

hexagonal closest-packed layer, or simply a closest-packed layer, and it can be shown that the circles in Fig. 23A occupy 90.7 per cent of the available space (Exercise 10). The unit cell of the plane lattice of this array is shown by broken lines in Fig. 23A. Note that each unit cell contains two kinds of void spaces, labeled B and C in Fig. 23B. Note